Reducing nonlinear dynamical systems via model reduction and machine learning

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Austin, Texas
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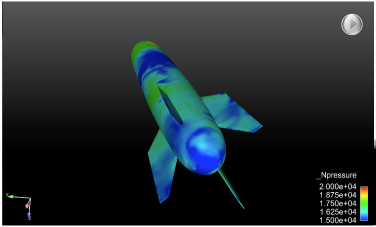
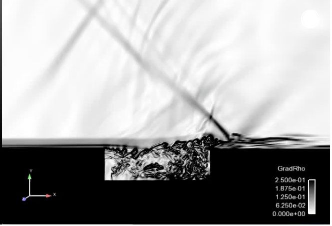
Goal: break computational barrier

High-fidelity computational models





+ Validated RANS/LES model: matches experiment to within 5%
- *Large scale*: 86 million cells; 200,000 time steps
- *High simulation costs*: 6 weeks; 5000 cores

Barrier

Many query applications

- Uncertainty quantification
- Design optimization

Nonlinear dynamical systems and many-query problems

Full-order model (FOM)

Full-order model
ODE

↓

time discretization

↓

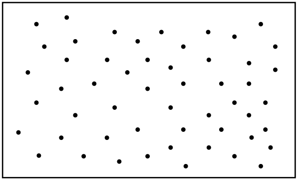
Full-order model
OΔE

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}; t, \boldsymbol{\mu});\ \boldsymbol{x}(0, \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu}),\ t \in [0, T],\ \boldsymbol{\mu} \in \mathcal{D}$$

$$\boldsymbol{r}^n(\boldsymbol{x}^n; \boldsymbol{\mu}) = 0, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}$$

Many-query problems

Goal: compute QoI $q(\boldsymbol{x}^n; \mu)$, $n = 1, \ldots, N$ for $\mu \in \mathcal{D}_{\text{eval}} \subset \mathcal{D}$



$\mathcal{D}_{\mathrm{eval}}$

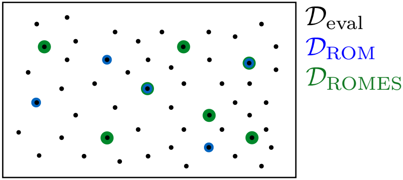
This is intractable with a large-scale FOM

Approach: ROM and ROMES

Reduce the FOM dimensionality and
quantify the introduced uncertainty

1. Reduced-order model (ROM)
   - **Goal**: low-dim dynamical system that accurately represents FOM
   - **Approach**: unsupervised machine learning and projection
   - \+ physics-based approximation
   - \+ can preserve special problem structure
   - \+ high speedups possible
2. Reduced-order model error surrogate (ROMES)
   - **Goal**: unbiased, low-variance statistical model of the ROM error
   - **Approach**: supervised machine learning (regression)
   - \+ more useful than error bounds (overpredict)
   - \+ quantifies ROM-induced epistemic uncertainty
   - \+ enables rigorous integration with UQ

Approach: leverage simulation data

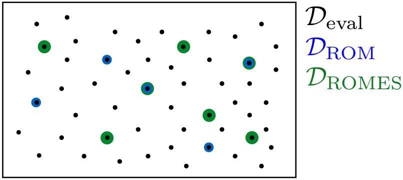


Offline:

1. **ROM training**: solve FOM for $\mu \in \mathcal{D}_{\text{ROM}} \subset \mathcal{D}_{\text{eval}}$
   - State and residual snapshots
2. **ROM construction**
   - *Unsupervised ML*: discover structure in ROM training data
   - *Projection*: reduce FOM dimensionality
3. **ROMES training**: solve ROM and FOM for $\mu \in \mathcal{D}_{\text{ROMES}} \subseteq \mathcal{D}_{\text{eval}}$
   - ROM error indicators
   - ROM QoI error
4. **ROMES construction**
   - *Supervised ML*: map ROM error indicators to ROM QoI error

Online: solve ROM + ROMES for remaining points in $\mathcal{D}_{\text{eval}}$

Approach: leverage simulation data



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3. **ROMES training**
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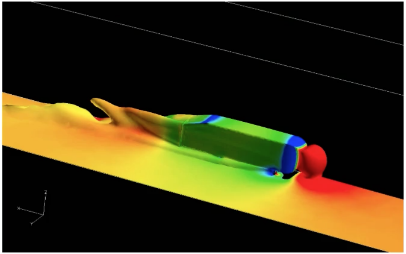
Online: solve ROM + ROMES for remaining points in $\mathcal{D}_{\text{eval}}$

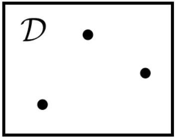
Collaborators: M. Barone (Sandia), H. Antil (GMU)

ROM training

$$\boldsymbol{r}^n(\boldsymbol{x}^n;\boldsymbol{\mu}) = 0, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}_{\mathrm{ROM}}$$

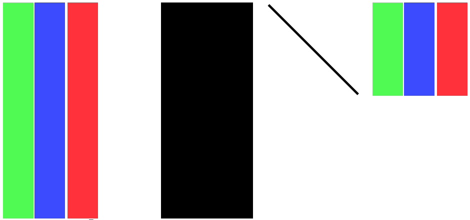
1 Collect 'snapshots' of the state (and residual)





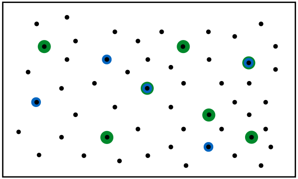
ROM construction: unsupervised machine learning

- Principal component analysis (i.e., POD)
  - Compute SVD: $[\,\mathbf{X}_1\ \mathbf{X}_2\ \mathbf{X}_3\,] = \mathbf{U}\ \boldsymbol{\Sigma}\ \mathbf{V}^T$



  - Truncate: $\boldsymbol{\Phi} = [\boldsymbol{u}_1\ \cdots\ \boldsymbol{u}_p]$
  - Repeat for residual to construct $\boldsymbol{\Phi}_R$
- Clustering
  - Construct sampling matrix $\boldsymbol{P}$ from residual data [C. et al., 2013]

Approach: leverage simulation data



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Online: solve ROM + ROMES for remaining points in $\mathcal{D}_{\mathsf{eval}}$

How to perform projection with state basis $\mathbf{\Phi}$?

Full-order model
ODE

↓

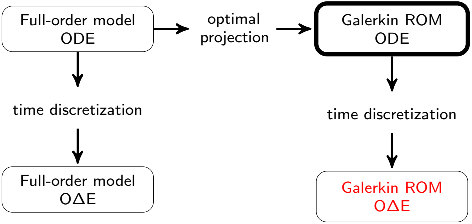
time discretization

↓

Full-order model
OΔE

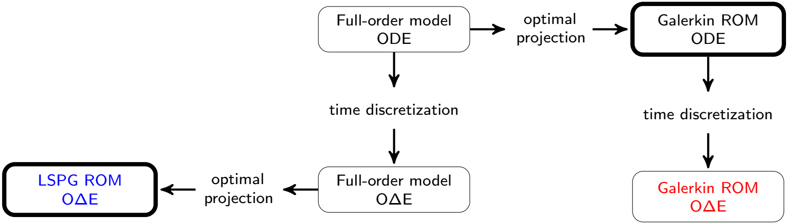
How to perform projection with state basis $\mathbf{\Phi}$?

- Optimize then discretize? (common)



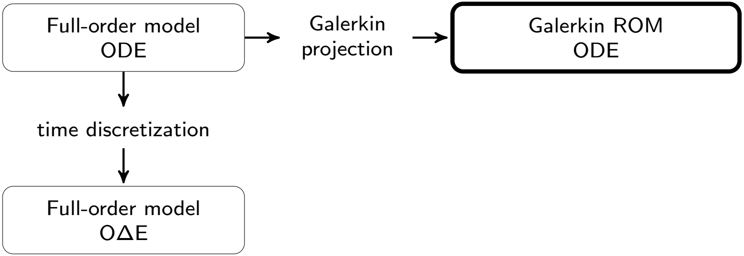
How to perform projection with state basis $\mathbf{\Phi}$?

- Optimize then discretize? (common)
- Discretize then optimize? (uncommon)



Comparative analysis: C, Barone, Antil, "Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction," Journal of Computational Physics, 330:693–734, 2017.

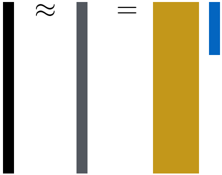
Galerkin ROM: first optimize



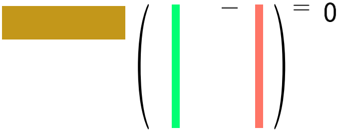
Galerkin ROM

- ODE: Galerkin projection on FOM ODE

1 $\boldsymbol{x}(t;\boldsymbol{\mu}) \approx \tilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) = \boldsymbol{\Phi}\hat{\boldsymbol{x}}(t;\boldsymbol{\mu})$



2 $\boldsymbol{\Phi}^T\left(\boldsymbol{f}(\tilde{\boldsymbol{x}}, t;\boldsymbol{\mu}) - \frac{d\tilde{\boldsymbol{x}}}{dt}\right) = 0$



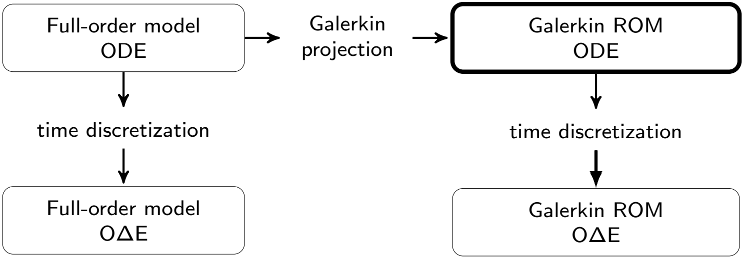
$$\frac{d\hat{\boldsymbol{x}}}{dt} = \boldsymbol{\Phi}^T\boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t;\boldsymbol{\mu}), \quad \hat{\boldsymbol{x}}(0;\boldsymbol{\mu}) = \boldsymbol{\Phi}^T\boldsymbol{x}^0(\boldsymbol{\mu}), \quad t \in [0, T], \quad \boldsymbol{\mu} \in \mathcal{D}$$

Theorem (Galerkin ROM: time-continuous optimality)

The Galerkin ROM velocity minimizes the time-continuous FOM residual:

$$\frac{d\tilde{\boldsymbol{x}}}{dt}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t;\boldsymbol{\mu}) = \arg\min_{\boldsymbol{v}\in range(\boldsymbol{\Phi})} \|\boldsymbol{v} - \boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t;\boldsymbol{\mu})\|_2^2.$$

Galerkin: first optimize, then discretize



Galerkin ROM

- ODE

$$\frac{d\hat{\boldsymbol{x}}}{dt} = \boldsymbol{\Phi}^T \boldsymbol{f}(\boldsymbol{\Phi}\hat{\boldsymbol{x}}, t; \boldsymbol{\mu}), \quad \hat{\boldsymbol{x}}(0) = \boldsymbol{\Phi}^T \boldsymbol{x}^0(\boldsymbol{\mu}), \quad t \in [0, T], \quad \boldsymbol{\mu} \in \mathcal{D}$$

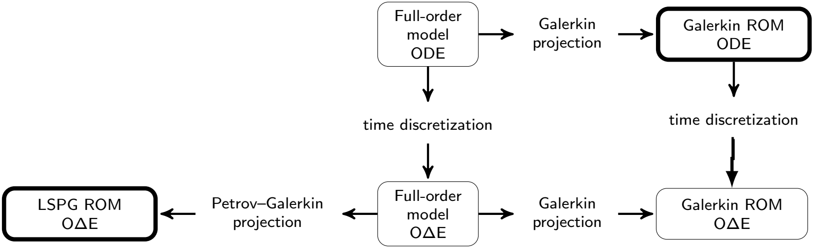
  + Continuous velocity $\frac{d\hat{\boldsymbol{x}}}{dt}$ is optimal

- OΔE

$$\boldsymbol{\Phi}^T \boldsymbol{r}^n (\boldsymbol{\Phi}\hat{\boldsymbol{x}}^n; \boldsymbol{\mu}) = 0, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}$$

  - Discrete state $\hat{\boldsymbol{x}}^n$ is not generally optimal

LSPG ROM: first discretize, then optimize



LSPG ROM

- FOM OΔE

$$\boldsymbol{r}^n(\boldsymbol{x}^n;\boldsymbol{\mu}) = 0, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}$$

- LSPG ROM OΔE:

$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}} \in \mathbb{R}^p} \|\boldsymbol{A}\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}};\boldsymbol{\mu})\|_2^2, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}$$

$$\Updownarrow$$

$$\boldsymbol{\Psi}^n(\hat{\boldsymbol{x}}^n;\boldsymbol{\mu})^T\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{x}}^n;\boldsymbol{\mu}) = 0, \quad n = 1, \ldots, N, \quad \boldsymbol{\mu} \in \mathcal{D}$$

  - $\boldsymbol{\Psi}^n(\hat{\boldsymbol{x}};\boldsymbol{\mu}) := \boldsymbol{A}^T\boldsymbol{A}\frac{\partial \boldsymbol{r}^n}{\partial \boldsymbol{x}}(\boldsymbol{\Phi}\hat{\boldsymbol{x}};\boldsymbol{\mu})$

  \+ Discrete solution is optimal

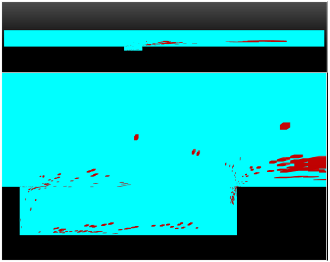
How to select weighting matrix $\boldsymbol{A}$? [C. et al., 2013]

$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\boldsymbol{A}\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}};\mu)\|_2^2$$

- Gappy POD approx of residual $\boldsymbol{r}^n \approx \tilde{\boldsymbol{r}}^n = \boldsymbol{\Phi}_R(\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}\boldsymbol{r}^n$

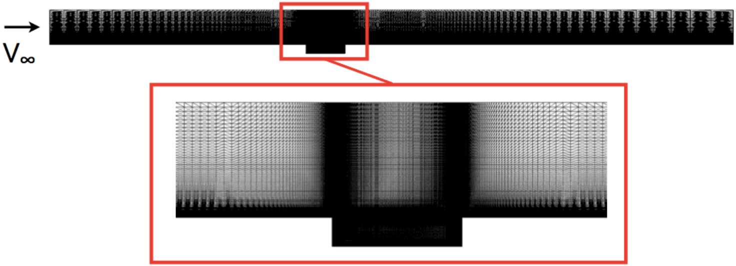
$$\hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\tilde{\boldsymbol{r}}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2 \Leftrightarrow \hat{\boldsymbol{x}}^n = \arg\min_{\hat{\boldsymbol{z}}\in\mathbb{R}^p} \|\underbrace{(\boldsymbol{P}\boldsymbol{\Phi}_R)^+\boldsymbol{P}}_{\boldsymbol{A}_{\mathrm{GNAT}}}\boldsymbol{r}^n(\boldsymbol{\Phi}\hat{\boldsymbol{z}})\|_2^2$$

- *Sample mesh*: Extract mesh subset needed to compute $\boldsymbol{P}\boldsymbol{r}^n$



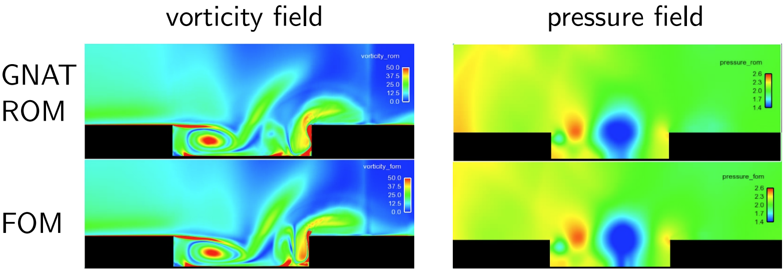
\+ Small problem size: can run on many fewer cores

Cavity-flow problem Collaborator: M. Barone (SNL)



- Unsteady, compressible Navier–Stokes
- DES turbulence model
- $M_\infty = 0.6$
- $\text{Re} = 6.3 \times 10^6$
- 1.2×10^6 degrees of freedom

GNAT performance ($t \leq 12.5$ sec)



+ $< 1\%$ error in time-averaged drag
+ Sample mesh: 4.1% nodes, 3.0% cells
+ 229x CPU-hour savings
  - FOM: 5 hour x 48 CPU
  - GNAT ROM: 32 min x 2 CPU
- Galerkin unstable

Why is LSPG more accurate than Galerkin? [C. et al., 2017]

Theorem (Local *a posteriori* bounds: BDF schemes)

If the following conditions hold:

1. $\exists \kappa > 0$ *such that* $\|\boldsymbol{f}(\boldsymbol{x}, \cdot; \cdot) - \boldsymbol{f}(\boldsymbol{y}, \cdot; \cdot)\|_2 \leq \kappa \|\boldsymbol{x} - \boldsymbol{y}\|_2$, $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^N$
2. Δt *small enough such that* $0 < h := |\alpha_0| - |\beta_0| \kappa \Delta t$
3. *A BDF scheme is employed for time integration, then*

$$\|\delta \boldsymbol{x}_G^n\| \leq \frac{1}{h} \|\boldsymbol{r}_G^n(\boldsymbol{\Phi} \hat{\boldsymbol{x}}_G^n; \boldsymbol{\mu})\|_2 + \frac{1}{h} \sum_{\ell=1}^{k} |\alpha_\ell| \|\delta \boldsymbol{x}_G^{n-\ell}\|$$

$$\|\delta \boldsymbol{x}_L^n\| \leq \frac{1}{h} \min_{\boldsymbol{y} \in range(\boldsymbol{\Phi})} \|\boldsymbol{r}_P^n(\boldsymbol{y}; \boldsymbol{\mu})\|_2 + \frac{1}{h} \sum_{\ell=1}^{k} |\alpha_\ell| \|\delta \boldsymbol{x}_L^{n-\ell}\|$$

- $\delta \boldsymbol{x}_G^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi} \hat{\boldsymbol{x}}_G^n$.
- $\delta \boldsymbol{x}_L^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi} \hat{\boldsymbol{x}}_L^n$

LSPG sequentially minimizes the time-local error bound

Can we use this bound for error estimation?

Time-global error bound [C. et al., 2017]

Theorem (Global *a posteriori* bounds: BDF schemes)

If the following conditions hold:

1. $\exists \kappa > 0$ *such that* $\|\boldsymbol{f}(\boldsymbol{x},\cdot;\cdot) - \boldsymbol{f}(\boldsymbol{y},\cdot;\cdot)\|_2 \leq \kappa \|\boldsymbol{x} - \boldsymbol{y}\|_2$, $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^N$
2. Δt *small enough such that* $0 < h := |\alpha_0| - |\beta_0|\kappa\Delta t$
3. *A BDF scheme is employed for time integration, then*

$$\|\delta \boldsymbol{x}_G^n\| \leq \frac{\gamma_1(\gamma_2)^n \exp(\gamma_3 t^n)}{\gamma_4 + \gamma_5 \Delta t} \max_{j\in\{1,\ldots,n\}} \|\boldsymbol{r}_G^j(\boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^j;\boldsymbol{\mu})\|_2$$

$$\|\delta \boldsymbol{x}_L^n\| \leq \frac{\gamma_1(\gamma_2)^n \exp(\gamma_3 t^n)}{\gamma_4 + \gamma_5 \Delta t} \max_{j\in\{1,\ldots,n\}} \min_{\boldsymbol{y}\in range(\boldsymbol{\Phi})} \|\boldsymbol{r}_P^j(\boldsymbol{y};\boldsymbol{\mu})\|_2$$

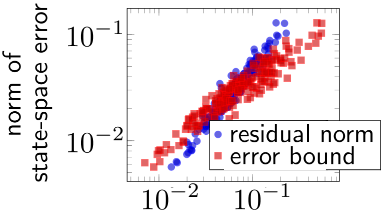
- $\delta \boldsymbol{x}_G^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_G^n$.
- $\delta \boldsymbol{x}_L^n := \boldsymbol{x}_\star^n - \boldsymbol{\Phi}\hat{\boldsymbol{x}}_L^n$

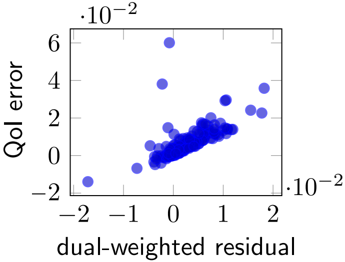
Global error bounds grow exponentially in time and overpredict the error

Deterministic: not amenable to integration with UQ

Idea: *construct accurate statistical error estimates from data*

Observation: ROMs generate error indicators that inform the error

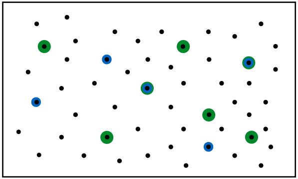




Goal: map error indicators (features) to the ROM error (response)

1. High-dimensional regression model (supervised ML)
   - maps error indicators to a prediction of the error
   - **methods**: random forest, support vector machine, k-NN
   - \+ enables many candidate error indicators to be considered
2. Gaussian-process model
   - maps regression-model output to a distribution over the error
   - \+ removes regression-model bias
   - \+ GP variance quantifies the ROM-induced epistemic uncertainty

Approach: leverage simulation data



Offline:

1. **ROM training**
2. **ROM construction**
3. **ROMES training**: solve ROM and FOM for $\mu \in \mathcal{D}_{\text{ROMES}} \subseteq \mathcal{D}_{\text{eval}}$
   - ROM error indicators
   - ROM QoI error
4. **ROMES construction**
   - *Supervised ML*: map ROM error indicators to ROM QoI error

Online: solve ROM + ROMES for remaining points in $\mathcal{D}_{\text{eval}}$

Collaborators: M. Drohmann, B. Freno (Sandia);
S. Trehan, L. Durlofsky (Stanford)

ROMES formulation [Drohmann and C., 2015, Trehan et al., 2017]

- FOM produces sequence of QoI values

$$\boldsymbol{\mu} \mapsto q_{\mathrm{FOM}}^n(\boldsymbol{\mu}) := q(\boldsymbol{x}^n(\boldsymbol{\mu}); \boldsymbol{\mu}), \quad n = 1, \dots, N$$

- ROM: produces sequence of QoI and error-indicator values

$$\boldsymbol{\mu} \mapsto q_{\mathrm{ROM}}^n := q(\boldsymbol{\Phi}\boldsymbol{x}^n(\boldsymbol{\mu}); \boldsymbol{\mu}), \quad n = 1, \dots, N$$
$$\boldsymbol{\mu} \mapsto \boldsymbol{\rho}^n(\boldsymbol{\mu}), \quad n = 1, \dots, N$$

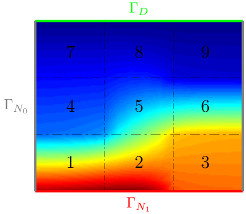
ROMES training:

1. Solve ROM and FOM for $\mu \in \mathcal{D}_{\mathrm{ROMES}}$
2. Training data: $\{(\boldsymbol{\rho}^n(\boldsymbol{\mu}), q_{\mathrm{FOM}}^n(\boldsymbol{\mu}) - q_{\mathrm{ROM}}^n(\boldsymbol{\mu})\}_{\boldsymbol{\mu}\in\mathcal{D}_{\mathrm{ROMES}}}$

ROMES construction:

1. Apply supervised ML to predict response from features
   - **Features**: error indicators $\boldsymbol{\rho}^n(\boldsymbol{\mu})$
   - **Response**: error $q_{\mathrm{FOM}}^n(\boldsymbol{\mu}) - q_{\mathrm{ROM}}^n(\boldsymbol{\mu})$
2. GP postprocessing to remove bias and quantify variance

Example 1: GP only, stationary problem [Drohmann and C., 2015]

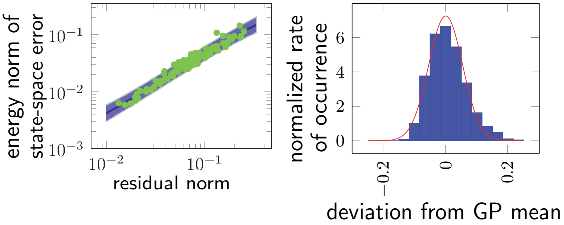


$$\triangle c(x;\boldsymbol{\mu})u(x;\boldsymbol{\mu}) = 0 \text{ in } \Omega \qquad \boldsymbol{x}(\boldsymbol{\mu}) = 0 \text{ on } \Gamma_D$$

$$\nabla c(\boldsymbol{\mu})\boldsymbol{x}(\boldsymbol{\mu}) \cdot n = 0 \text{ on } \Gamma_{N_0} \qquad \nabla c(\boldsymbol{\mu})\boldsymbol{x}(\boldsymbol{\mu}) \cdot n = 1 \text{ on } \Gamma_{N_1}$$

- **Inputs**: $\boldsymbol{\mu} \in [0.1, 10]^9$ define diffusivity c in subdomains
- **ROM**: RB–Greedy [Patera and Rozza, 2006]

Error: energy norm of state-space error
Error indicator: residual norm

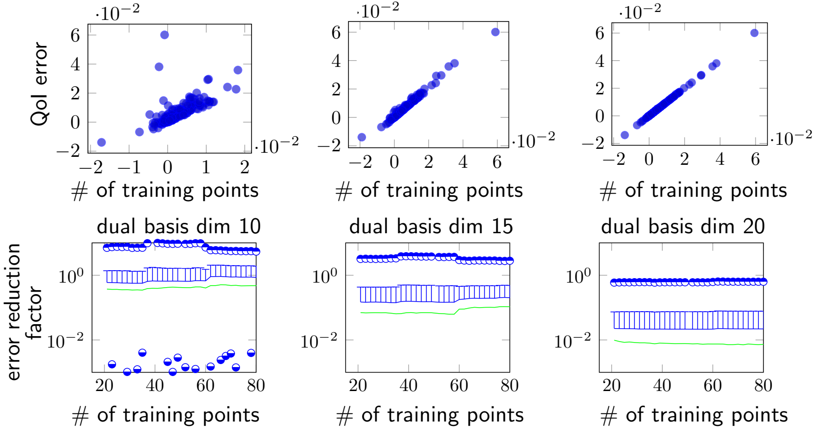


+ Unbiased, low-variance model of the error
+ Numerically validated
- Error bound overprediction as high as 8.0

Error: error in temperature at a point

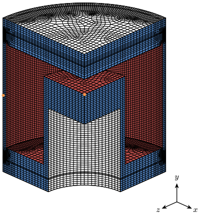
Error indicator: dual-weighted residual

$$\hat{\boldsymbol{y}}(\boldsymbol{\mu})^T \boldsymbol{Y}^T \boldsymbol{r}(\boldsymbol{\Phi}\hat{\boldsymbol{x}};\boldsymbol{\mu}) \text{ with } \boldsymbol{Y}^T \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{x}}(\boldsymbol{\Phi}\hat{\boldsymbol{x}};\boldsymbol{\mu})^T \boldsymbol{Y}\hat{\boldsymbol{y}}(\boldsymbol{\mu}) = -\boldsymbol{Y}^T \frac{\partial q}{\partial \boldsymbol{x}}(\boldsymbol{\Phi}\hat{\boldsymbol{x}};\boldsymbol{\mu})$$



+ Uncertainty control: lower variance as columns added to $\boldsymbol{Y}$
+ Error can be reduced by up to two orders of magnitude

Example 2: ML and GP, stationary problem [Freno and C, 2017]

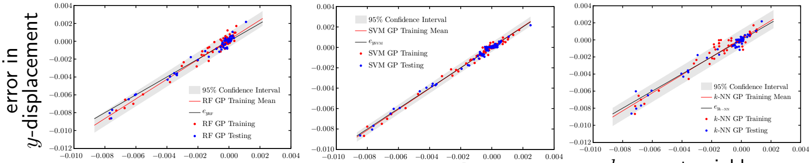


Predictive Capability Assessment Project (PCAP)

- Mechanical response
- 2.8×10^5 degrees of freedom
- **Inputs**: $\boldsymbol{\mu} \in [50\text{ GPa}, 100\text{ GPa}] \times [0.2,\ 0.35]$ define tube elastic modulus and Poisson ratio
- **QoI**: displacement of node of interest (orange)
- **ROM**: POD–Galerkin with $|\mathcal{D}_{\mathrm{ROM}}| = 8$
- **ROMES**: 150 data points ($|\mathcal{D}_{\mathrm{ROMES}}| = 30$ and five ROM basis dimensions)

Error: error in y-displacement at a point

Error indicators: 5000 elements of residual, input parameters

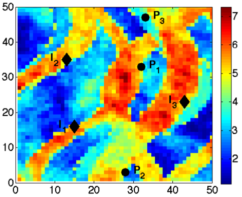


random forest error prediction | support vector machine error prediction | k-nearest neighbors error prediction

+ ML methods yield low-variance error predictions
+ ML methods amenable to large number of error indicators
+ Gaussian process removes regression-model bias

Example #3: ML and GP, nonlinear dynamical system

[Trehan et al., 2017]

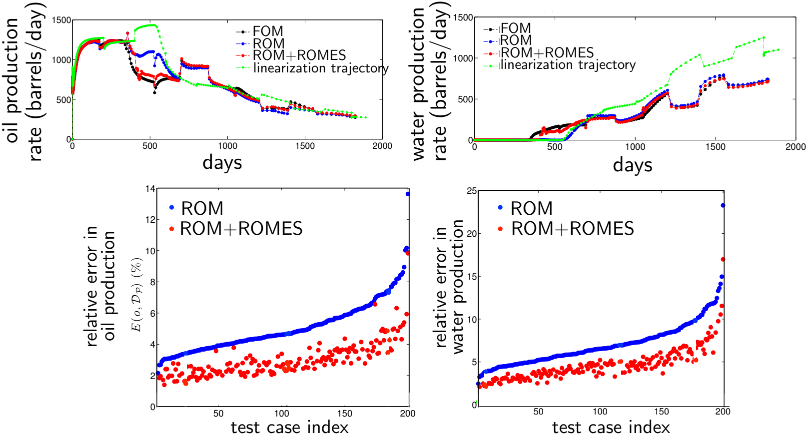


Permeability field with injection I_j and production P_j wells

- Two-phase oil–water system in porous medium (Darcy's law)
- 5×10^3 degrees of freedom
- **Inputs**: time-varying bottom-hole pressure (BHP) at injector wells
- **QoI**: oil/water production rates
- **ROM**: POD–TPWL with $|\mathcal{D}_{\text{ROM}}| = 3$
- **ROMES**: $|\mathcal{D}_{\text{ROMES}}| = 200$

Error: phase flow rates at production well

Error indicators: 168 application-specific quantities



+ ROMES correction significantly improves ROM prediction

Summary: ROM and ROMES

Reduce the FOM dimensionality and quantify the introduced uncertainty

1. Reduced-order model (ROM)
   - **Goal**: low-dim dynamical system that accurately represents FOM
   - **Approach**: unsupervised machine learning and projection
   + physics-based approximation
   + can preserve special problem structure
   + high speedups possible
2. Reduced-order model error surrogate (ROMES)
   - **Goal**: unbiased, low-variance statistical model of the ROM error
   - **Approach**: supervised machine learning (regression)
   + more useful than error bounds (not sharp)
   + quantifies ROM-induced epistemic uncertainty
   + enables rigorous integration with UQ

Questions?

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